Atmospheric Reactivity of Volatile Organic Compounds (VOCs)

Subcontractor

University of California, Riverside

Principal Investigator

William P.L. Carter
College of Engineering—
Center for Environmental Research
and Technology (CE-CERT)
University of California
Riverside, CA 92521
(909) 781-5797

DOE Project Manager

Michael Gurevich
U.S. Department of Energy
CE-332, MS 6A-116/Forrestal
1000 Independence Avenue, SW
Washington, DC 20585
(202) 586-6104

NREL Technical Monitor

Brent Bailey
NREL
1617 Cole Boulevard
Golden, CO 80401
(303) 275-4468

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Scott Montgomery (303) 275-3193

Objectives

- Provide environmental chamber data to reduce uncertainties in estimates of atmospheric ozone impacts of current and alternative fuel vehicle emissions
- Fill gaps in the environmental chamber database for evaluating gas-phase chemical mechanisms for ambient air quality models
- Evaluate effects of environmental conditions on ozone impacts of VOCs.

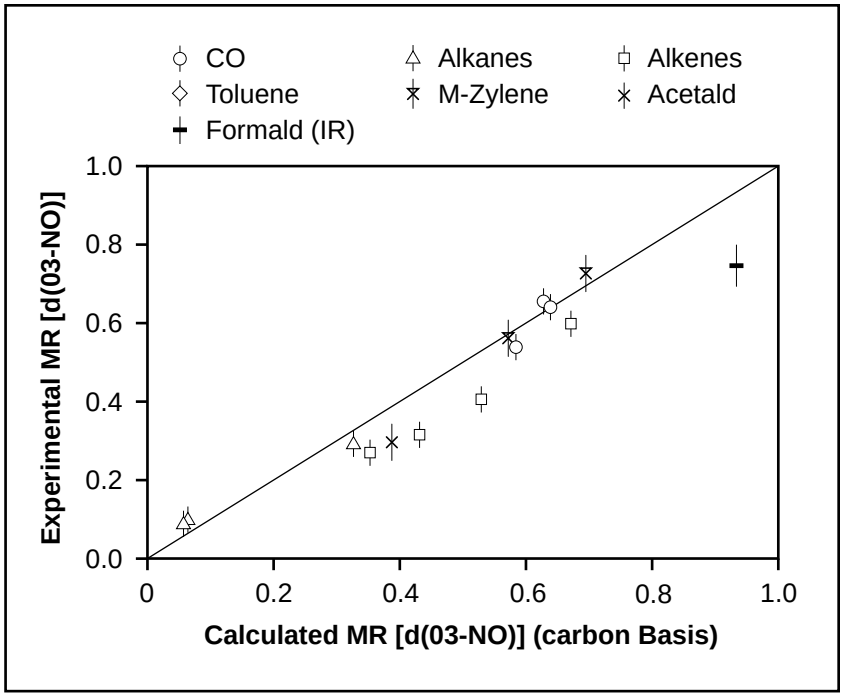

Figure 1:

Approach

- Use environmental chamber experiments to measure changes in ozone formation and VOC consumption rates caused by adding representative VOCs to simulated photochemical smog systems. Vary NO_x to total VOC ratios and the composition of the other VOC pollutants (base reformulated oxygenated gasoline [ROG] surrogate).
- Conduct experiments with relatively high NO_x/base ROG rations to test the Maximum Incremental Reactivity (MIR) scale. Conduct experiments with low ratios to measure the effect of the VOC on ultimate ozone-forming potential.
- Conduct experiments with simple base ROG surrogates to provide the most sensitive and straightforward test of the mechanism. Conduct experiments with more complex surrogates to more closely respond to the ambient conditions.
- Vary the light source to test our understanding and ability to predictively model the photolytic processes that cause photochemical smog formation.

Accomplishments

- Conducted reactivity experiments under high NO_x/base ROG conditions and using a simple ROG surrogate and a blacklight light source for a total of 39 VOCs. These included representative alkalines, aromatics, and oxygenates.
- Conducted reactivity experiments for nine VOCs with varying NO_x and ROG surrogate compositions.
- Constructed a new environmental chamber with a xenon arc light source to assess the effects of varying light source, which represents more closely the spectrum of sunlight than do the blacklights. Conducted preliminary runs with simple model systems and compared them with data using other chambers.
- Used the data to evaluate the chemical mechanism previously used to calculate the MIR reactivity scale and evaluate an updated version of the mechanism. The mechanisms simulated the results reasonably well, but there were some inconsistences between model predictions and experimental data.

Future Direction

We are conducting the following:

- A more comprehensive set of reactivity experiments using the xenon light source to assess light source effects on experimental reactivity data
- Experiments to assess effects of humidity on environmental chamber results
- Experiments to provide data needed to improve model predictions of reactivity differences among aromatic isomers.

Publications

Carter, W.P.L., J.A. Pierce, I.L. Malkina, D. Luo, and W.D. Long. (1993.) *Environmental Chamber Studies of Maximum Incremental Reactivities of Volatile Organic Compounds*, NREL Final Report.

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